

Listing of the Claims

1. (previously presented) A computer-implemented method of comparing molecules, comprising:
 - providing a set of field points representing field extrema of a first molecule, wherein each field point has a position and a field size value;
 - determining at the position of each of the field points of the first molecule the field of a second molecule to obtain a set of field sample values; and
 - combining the field sample values with the field size values to provide a score indicative of the field similarity of the first molecule to the second molecule.
2. (original) The method of claim 1, wherein the field sample values are determined by applying the position of each of the field points to a field definition formula.
3. (previously presented) The method of claim 1, wherein the field sample values are determined by calculating the field by interpolation from a pre-calculated grid of field size values around the second molecule.
4. (previously presented) The method of claim 1, wherein, during the combining, the field size values are transformed to scaled field size values such that two field points having a first field size value give the same contribution to the score as one field point having a field size value twice the first field size value.
5. (original) The method of claim 4, wherein the scaled field size values have the magnitude of the square root of the absolute field size values and the sign of the field size values.
6. (previously presented) The method of claim 1, wherein combining the field sample values and the field size values involves obtaining their product.

7. (previously presented) The method of claim 1, further comprising:
providing a second set of field points representing field extrema of the second molecule, wherein each field point has a position and a field size value;
determining at the position of each of the field points of the second set the field of the first molecule to obtain a further set of field sample values;
combining the further field sample values with the field size values of the field points of the second set to obtain a further score, wherein the further score is indicative of the field similarity of the second molecule to the first molecule; and
combining the further score with the score of the field similarity of the first molecule to the second molecule to provide an aggregate score.

8. (original) The method of claim 7, wherein the further field sample values are determined by applying the position of each of the field points of the second set to a field definition formula.

9. (previously presented) The method of claim 7, wherein the further field sample values are determined by calculating the field by interpolation from a pre-calculated grid of field size values around the first molecule.

10. (previously presented) The method of claim 7, wherein combining the further field sample values and the field size values involves obtaining their product.

11. (previously presented) The method of claim 1, wherein the field size values are energy values.

12. (previously presented) The method of claim 1, wherein the field extrema are field minima.

13. (previously presented) A computer interpretable recording medium bearing a set of instructions executable by a computer for carrying out the process of claim 1.

14. (cancelled)

15. (cancelled)

16. (previously presented) A computer apparatus configured to carry out the method of claim 1.